

Surface and bulk properties of ballistic deposition models with bond breaking

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We introduce a new class of growth models, with a surface restructuring mechanism in which impinging “hot” atoms may dislodge suspended particles (deposited following the ballistic deposition rule), previously aggregated on the same column in the deposit. The flux of these “hot” particles is controlled through a probability p . These systems present a crossover, for small values of p , from random to correlated (KPZ) growth of surface roughness, which is studied through scaling arguments and Monte Carlo simulations on one- and two-dimensional substrates. We show that the characteristic time of crossover t_{\times} scales with p according to $t_{\times} \sim p^{-y}$ with $y = (n + 1)$ and that the interface width at saturation W_{sat} scales as $W_{sat} \sim p^{-\delta}$ with $\delta = (n + 1)/2$, where n is either the maximal number of bonds broken or of suspended particles that may be dislodged. Thus, the exponents $y = 1$ and $\delta = 1/2$ or $y = 2$ and $\delta = 1$ found in all previous works, are not universal. Using scaling arguments, we show that the bulk porosity P of the deposits scales as $P \sim p^{y-\delta}$ for small values of p . This general scaling relation explains previous results present in literature and is confirmed by our numerical simulations.

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I. INTRODUCTION

The morphology and evolution of the surface and porous structure in thin-film growth has been a subject of extensive theoretical and experimental interest [1, 2]. From a theoretical side, a number of surface growth models have been proposed, being the ballistic deposition (BD) model [3] one of the first. The BD model was initially formulated to explain sedimentary rock formation, but has also been extensively studied as a model of low-temperature thin-film growth and surface roughening [2]. In the last decades, the surface properties of the BD model were widely studied (see refs. [1, 2, 4] and references therein) and it is believed to be in the Kardar-Parisi-Zhang (KPZ) [5] universality class. More recently, some efforts were also devoted to understand its bulk structure [6, 7]. Furthermore, some variations of the BD model were also considered. Some examples are ballistic deposition with oblique incidence of particles [8, 9], slippery BD [7, 10, 11], and competitive growth models in which particles are deposited following probabilistically either BD or other deposition rules [12–20].

In all models above, after deposition, the particles are permanently aggregated in the deposit and do not change their positions (limited mobility models). Here, we study a different class of BD-like models in which aggregated particles can be rearranged in the deposit due to bond breaking, hereafter referred to bond-break ballistic deposition (BBBD) models. More specifically, BD particles are deposited with probability p and “random deposition-like” (RD-like) particles with probability $1 - p$. When a “RD-like” particle impinges over suspended particles, their bonds can break and they fall together until reaching the next top of the column. We consider the case where up to n bonds can break (BBBD models) and

the case where up to n suspended particles can change their positions, independently of the number of lateral bonds (BBBD models). When bonds do not break, the “RD-like” particle is deposited on the top of the column (simple RD rule).

In a very simplified way, a ballistic deposition models a low-temperature system (with thermally activated diffusion process inoperative) where all impinging atoms immediately dissipate the energy released upon formation of the atom-surface bond. However, in general, such energy could be not immediately dissipated and the impinging “hot” atom may perform/produces some transient movements at surface. Some examples are *downward funneling*, *transient mobility*, *knockout* and *cascading knockdown* of adatoms, which are processes responsible for smooth the surface in low-temperatures [21–23]. In the last one, the “hot” atom dislodge previously deposited atoms that are only partially supported (suspended atoms), and they can move together to the “bottom valley”. Such mechanism induces the formation of a more compact film, eliminating overhangs at the surface. Thus, the bond break in the BBBD models may represents (in a simplified way) this concerted multiatom dynamics.

Since for $p = 0$ and $p = 1$ the BBBD models behave as plain RD and BD models, respectively, they present a competition from random to correlated (KPZ) growth. In systems with this kind of competition, the scaling behavior of the roughness (or interface width) W is given by the empirical form [15, 20]:

$$W \sim \frac{L^{\alpha_{BD}}}{p^{\delta}} F\left(\frac{t/p^{-y}}{L^{z_{BD}}}\right) \quad (p \rightarrow 0), \quad (1)$$

where $F(u)$ is a scaling function which behaves as $F(u) \sim u^{\beta_{BD}}$ with $\beta_{BD} = z_{BD}/\alpha_{BD}$ for $u \ll 1$ and $F(u) \sim$

const. for $u \gg 1$. α_{BD} is the roughness, β_{BD} is the growth and z_{BD} is the dynamical exponents of the BD model. In general, δ and y are exponents dependent of the correlated model and independent of the dimensionality of the system. Results for several competitive models [14, 19, 20, 24] suggests that the exponents δ and y are not directly linked to the universality class of the correlated process and can be separated in two groups: the first one including solid-on-solid (SOS) correlated models, for which $\delta = 1$ and $y = 2$; and the second one including correlated models with lateral aggregation (ballistic-like models), for which $\delta = 1/2$ and $y = 1$. These pair of exponents are claimed to be universal, i. e., every model with a crossover from random to correlated growth would present one of those pair of exponents [20]. As we will show below, it is not the case, and for ballistic-like models the exponents assume the general values $\delta = (n+1)/2$ and $y = n+1$, where n is the maximal number of either bonds broken or suspended particles dislodged.

Beyond the surface properties, in practical applications the internal structure of the material (beneath the surface) may be also relevant to determine mechanical and transport properties of the system. In this context, some recent works have focused also the porous (bulk) structure [6, 25–28]. Here, we study the bulk properties of the deposits generated by the BBBD models. Using scaling arguments, we show that the porosity P of the deposits scales as $p^{y-\delta}$ for small p , where δ and y are the exponents defined above (Eq. 1). Thus, this work advances over previous ones, which only relate P with p [11, 27, 28], since here we relate directly the scaling exponents of the amplitudes of surface roughness with that of bulk quantities.

The rest of this work is organized as follows. In Section II we describe the BD models with bond-breaking introduced here. In Section III we present the scaling theory to explain the behaviors of surface and bulk properties for small values of the probability p . Numerical results for the BBBD and BBBDS are presented in Subsections IV A and IV B, respectively. Final discussions and conclusions may be found in Section V.

II. THE MODELS

In the BBBD models considered here, the impinging particle, following a vertical trajectory, can either dissipate all its energy at collision sticking at the point where it first contacts the surface (BD rule) or transfer energy to the particles below it, dislodging these particles if they are suspended. In this case, the particles (impinging and dislodged) are deposited at the next top below them. Two kinds of models were considered when dislodging particles: i) accounting the number of bonds breaking (BBBDB models); and ii) accounting the number of suspended particles dislodged (BBBDS models). In the first case, up to n bonds can break, and, in the second, up to n suspended particles can be dislodged. When it is not

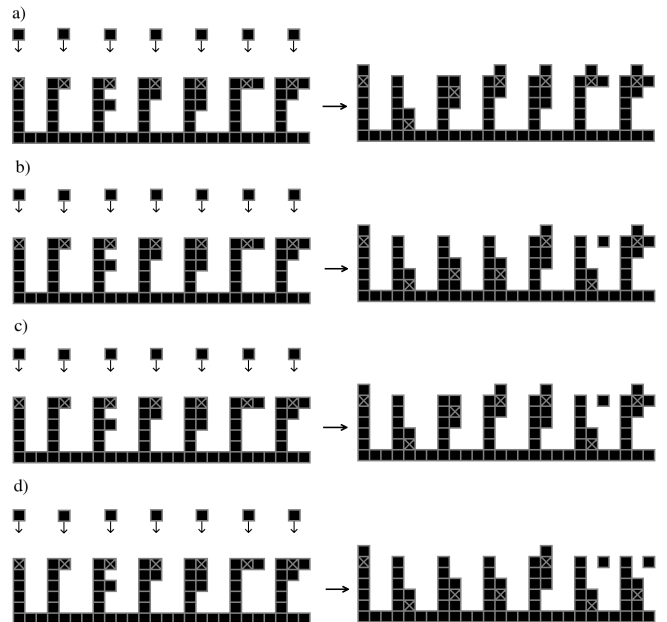


FIG. 1: Illustration of the bond breaking rules (happen with probability $1 - p$) for the BBBDB models with a) $n = 1$ and b) $n = 2$, and BBBDS models with c) $n = 1$ and d) $n = 2$. Deposits before (left) and after (right) deposition of seven particles are shown.

possible to dislodge particles, the impinging particle is deposited at the top of the incidence column (RD rule).

In both classes of models, a particle is dropped vertically at a randomly selected column i and sticks on the first site encountered on the surface that is nearest-neighbor of an already deposited particle (BD rule) with probability p . In BBBDB models, with probability $1 - p$, the number k of bonds of the target (top most) particle at column i is determined. If $k > n$ the incident particle is deposited at the top of the column, without bond break. If $k = n$ the target particle is unbounded and slide down vertically (together with the incident particle) to the next local minimum. Note that, in most cases there is no movement of the target particle because it is not suspended (there is a particle just below it). If $k < n$, particles below the target one could be unbounded (and dislodged also), provided that the total number of bonds breaking are smaller or equal to n . Figs. 1 (a)-(b) illustrate this growth rule for $n = 1$ and $n = 2$.

In BBBDS models, with probability $1 - p$, the number k of *consecutive* suspended particles in column i is counted, starting from the top. If $k > n$, the incident particle is deposited at the top of the column, without bond break. If $k = n$ the block of n suspended particles and the incident one slide down vertically to the next top. If $k < n$, suspended particles below the first suspended block of particles may also be dislodged, until a block of size smaller or equal n be attained. Figs. 1 (c)-(d) illustrate this growth rule for $n = 1$ and $n = 2$.

For $n = 0$, BBBDB and BBBDS models reduce to the simpler RD-BD model proposed by Horowitz and Albano [15]. Thus, the RD-BD model is a particular case of the BBBD models, referred here just as BBBD0 model. Simulations of this model showed that it exhibits a crossover, at a characteristic time t_x , from RD to KPZ growth and gave $\delta \simeq 1/2$ and $y \simeq 1$ in $d = 1 + 1$, $d = 2 + 1$, and $d = 3 + 1$ dimensions [15] (see also [20] and references therein). For completeness, we present below simulations results of the BBBD0 model, that are consistent with the results above. Moreover, we present also results for the bulk properties of this model, which was not studied yet.

III. SCALING THEORY

Different scaling arguments have already explained the values of the exponents δ and y obtained in simulations of several competitive lattice models [18–20]. For the BBBD0 (RD-BD) model, the basic argument is that, for small values of p , the average time for a correlated BD event (which involves lateral aggregation with probability p) to take place at a given column is $\tau \sim 1/p$. During the period τ , particles on average are directly deposited onto the surface according to the simple RD rule and the local height increases by $\sqrt{\tau}$. Thus, the BBBD0 model can be viewed (for small p) as a limiting BD model in which time scales as $\tau \sim 1/p$ while roughness scales as $W \sim \sqrt{\tau} \sim 1/p^{1/2}$. This explains the scaling function given by Eq. (1) and the conjectured values $\delta = 1/2$ and $y = 1$ for this model. This argument also gives the relationship $\delta = y/2$ which is valid for all models with crossover from RD to some correlated deposition dynamics [20].

For others BBBD models, we expect a similar argument. However, due to the bond breaking processes, which is frequent for small p , a single BD event is not sufficient to introduce lateral aggregation and cancel the random fluctuation of the heights. In order to ensure lateral growth, it is necessary that more BD particles fall (consecutively) at the same column. For example, if one suspended particle could be dislodged in the deposit, two consecutive BD events are needed to produce a correlated growth, giving $\tau \sim 1/p^2$ and $W \sim \sqrt{\tau} \sim 1/p$, and the exponents $\delta = 1$ and $y = 2$. In general, if n bonds could break, or n suspended particles could be dislodged, it is necessary $n + 1$ ballistic particles to introduce correlations, which leads to $\tau \sim 1/p^{n+1}$ and $W \sim \sqrt{\tau} \sim 1/p^{(n+1)/2}$, and thus to the expected exponents

$$\delta = (n + 1)/2 \quad \text{and} \quad y = (n + 1) \quad (2)$$

for these models, in any substrate dimension. It is worth mentioning that in all previously studied competitive models involving RD and solid-on-solid (SOS) correlated models (for example, RD-RSOS (restricted SOS) [19] and RD-RDSR (random deposition with surface relaxation) [20]), exponents $\delta = 1$ and $y = 2$ were found. In contrast,

systems with RD and BD-like models (for example, the BBBD0 model [15, 20]) have the exponents $\delta = 1/2$ and $y = 1$. This resulted in a classification of the models in two groups: RD-SOS models (with $\delta = 1$ and $y = 2$) and RD-BD like models (with $\delta = 1/2$ and $y = 1$) [14, 19, 20, 24], and these two sets of exponents were claimed to be universal (the only two pair of possible values) in random-to-correlated crossover [20]. Our results shows that for RD-BD like models, the exponents would be $\delta = (n + 1)/2$ and $y = n + 1$, that gives $\delta = 1/2$ and $y = 1$ in the case $n = 0$ (no bond breaking) already considered.

It is possible to extend the scaling arguments presented above to explain the behavior of the bulk porosity P of the deposits, for small p . The porosity P is the fraction of empty lattice sites inside the deposit:

$$P = \frac{V_P}{V_S + V_P} \quad , \quad (3)$$

where V_P is the total volume of the pores (vacant sites) and V_S is the total volume of the solid (particles) in the deposit. For small p , the pores are narrow in the horizontal direction (~ 1 site width) but vertically high. A typical height difference between neighboring columns is of order $\sqrt{\tau} \sim p^{-\delta}$ for small p and, thus, the lateral aggregation events create pores with volume of order $p^{-\delta}$. After V_S depositions, the average number of pores created is of order $p^y V_S$, since the characteristic time in which correlations between neighboring columns are built scales as $\tau \sim p^{-y}$. Thus, we obtain $P \sim p^\Delta$, with $\Delta = y - \delta$, which must be valid in any substrate dimension. It is worth mentioning that for the bidisperse BD model (for which $\delta = 1/2$ and $y = 1$) the scaling behavior $P \sim p^{1/2}$ was obtained in Ref. [27], consistent with the most general scaling above. Here, we must expect the exponents $\Delta = (n + 1)/2$ for the BBBD models.

IV. NUMERICAL RESULTS

The following results are for simulations on $d = 1 + 1$ substrates of sizes in the range $L = 64 - 1024$, and $d = 2 + 1$, with sizes in the range $L = 8 - 128$. In both cases, we assume periodic boundary conditions. Averages over 400 – 1000 different runs were made.

A. BBBDB models

Figure 2 shows plots of the roughness W versus time t obtained for the BBBDB1 model for two values of p , in $d = 1 + 1$. For short times, say $t < t_x$, the growth is dominated by the RD process and $W \sim t^{1/2}$ for $p < 1$. At intermediate times, $t_x < t < t_s$, correlations have developed and the BD process dominate giving $W \sim t^\beta$. Using data for different lattice sizes and extrapolating to $L \rightarrow \infty$, we obtained growth exponents $\beta \approx 0.33$ for every studied value of $p > 0$ in $d = 1 + 1$. This procedure

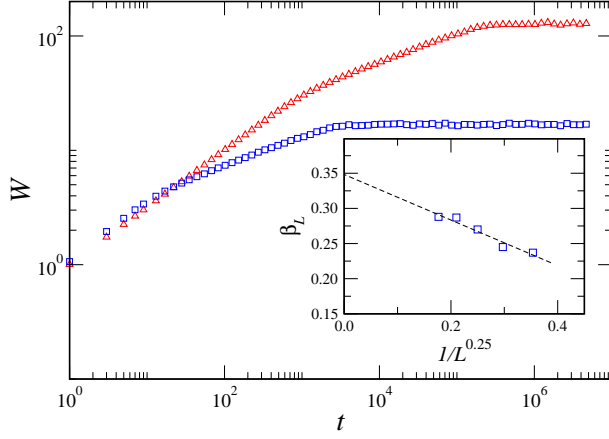


FIG. 2: Roughness W versus time t for the BBBDB1 model with $p = 0.05$ and $p = 0.5$, for a system size $L = 512$. The inset shows effective growth exponents β_L against $(1/L)^{0.25}$ for $p = 0.5$. The linear fit gives the extrapolated value $\beta_\infty = 0.35 \pm 0.03$.

to obtain $\beta_{L \rightarrow \infty}$ is illustrated in the inset of Fig. 2, for $p = 0.5$. This asymptotic exponent is consistent with the expected KPZ one ($\beta = 1/3$) and with previous simulation results for the BD model in $d = 1 + 1$ [4]. Finally, for $t > t_s$ the correlations can no longer develop due to the geometrical constraint of the lattice size and saturation occurs. Similar $W \times t$ behaviors are found in all models studied here and in other systems with random to KPZ crossover [20, 27].

Bellow, we present results for the BBBD0 and BBBDB models with $n = 1$ and 2, in $d = 1 + 1$ and $d = 2 + 1$ substrates.

In Fig. 3(a) the saturation roughness W_{sat} as a function of p is shown. As expected, for a given p , a larger n implies a larger W_{sat} . For small values of p , straight lines are observed in the log-log plot, in agreement with Eq. (1), and the best fits give the exponent δ in excellent agreement with the scaling theory of Sec. III (see Table I).

The crossover times t_\times , for different values of p , are shown in Fig. 3(b). The straight lines in the log-log plot, for small values of p , show that the scaling behavior $t_\times \sim p^{-y}$ from Eq. 1 is satisfied and yields exponents y in great accordance with the predicted ones, as summarized in Table I.

As the roughness, the porosity of the aggregate grows in time and attain a stationary value P for large t . Fig. 3(c) shows this stationary porosity as a function of the probability p . A good scaling behavior is found for small p and the exponents Δ obtained are consistent with the expected values (see Table I).

The results above are for substrate sizes $L = 128$ (in $d = 1 + 1$) and $L = 32$ (in $d = 2 + 1$). We notice that we have to work with small system sizes because the saturation times for $p \ll 1$ became very long for large n . However, it is not a limitation since, as pointed out in

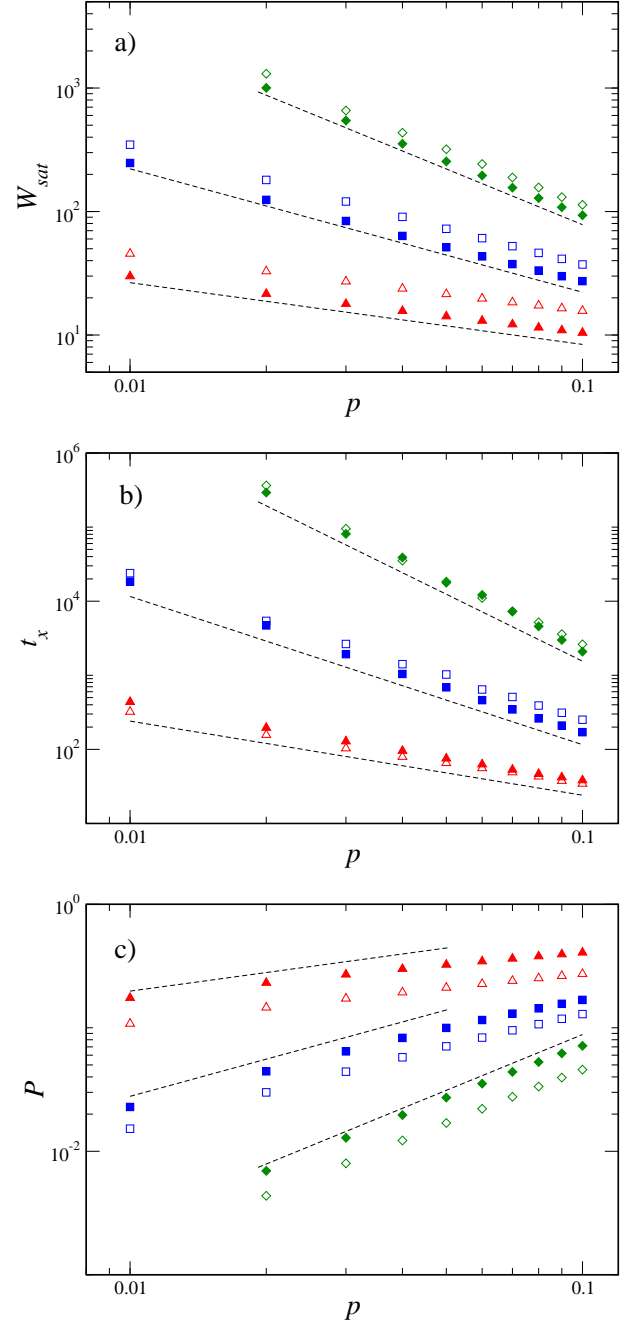


FIG. 3: a) Saturation roughness W_{sat} , b) crossover times t_\times and c) porosity P versus probability p for the BBBDB models with $n = 0$ (red triangles), $n = 1$ (blue squares) and $n = 2$ (green diamonds). Data for simulations on $d = 1 + 1$ substrates of size $L = 128$ (open symbols) and $d = 2 + 1$ with $L = 32$ (full symbols) are shown. In order to improve visualization, in (a) and (c) the data for $n = 1$ and 2 in $d = 2 + 1$ are, respectively, multiplied (shifted up) and divided (shifted down) by 1.5. The straight lines have slopes (from the bottom to top): a) $-1/2$, -1 and $-3/2$, b) -1 , -2 and -3 , and c) $3/2$, 1 and $1/2$.

Ref. [20], the exponents δ and y have weak finite-size

	BBBD0	BBBDB1	BBBDB2
y	0.98(3)	1.96(5)	3.0(1)
δ	0.46(5)	0.98(3)	1.50(2)
Δ	0.43(3)	0.97(4)	1.48(4)
y	1.02(5)	2.02(3)	3.03(7)
δ	0.47(4)	0.98(3)	1.49(3)
Δ	0.40(5)	0.96(5)	1.50(3)

TABLE I: Amplitude exponents y and δ and porosity exponent $\Delta = y - \delta$ for $d = 1 + 1$ (top) and $d = 2 + 1$ (bottom).

effects. In fact, from simulations for other system sizes (smaller and larger in same cases) we obtain exponents close to that shown in Table I.

Summing up, our numerical results are consistent with the roughness scaling relation (1), and the exponents δ , y and Δ obtained confirms the exact values from the scaling theory presented above.

B. BBBDS models

We made simulations of BBBDS models with $n = 1$, 2 and 3 in $d = 1 + 1$ and $d = 2 + 1$ dimensions. As discussed above, the roughness evolution with time has a similar behavior to the one shown in Fig. 2, for all BBBDS models with $p < 1$.

In BBBDS models, more particles are dislodged, for a given n , than in BBBDB ones (see Fig. 1). Thus, in the former the correlations develop more slowly, what makes the crossover times and the saturation roughness larger. On the other hand, the porosity is smaller in BBBDS models, since more particles are compactified by dislodgment. For example, for $n = 1$ and fixed L and p , we found $W_{sat}^{BBBDS}/W_{sat}^{BBBDB} \approx t_x^{BBBDS}/t_x^{BBBDB} \approx 1.5$ in $d = 1 + 1$ and ≈ 3 in $d = 2 + 1$, while $P^{BBBDB}/P^{BBBDS} \approx 1.2$ in $d = 1 + 1$ and ≈ 1.5 in $d = 2 + 1$.

In Fig. 4 we show the saturation roughness W_{sat} , the crossover time t_x and the stationary porosity P as functions of p . As in BBBDB models, we found here good scaling behaviors, for small p , consistent with the scaling relation given in Eq. 1. The exponents y , δ and Δ are in great agreement with the expected ones, as shown in Table II.

The data above are for substrate sizes $L = 128$ in $d = 1 + 1$. In $d = 2 + 1$ we have $L = 32$ for $n = 1$ and 2, and $L = 16$ for $n = 3$. Exponents obtained for other system sizes are close to the ones in Tab. II, again, showing that such exponents have negligible finite-sizes effects. For $n = 3$, the large crossover and saturation times restrains our simulations to substrate sizes $L \leq 16$ in $d = 2 + 1$. For these sizes, there is not a clear KPZ region in the $W \times t$ curves. In other words, the crossover and saturation times became very close, so that it is not possible to determine the former one. Thus, we are not

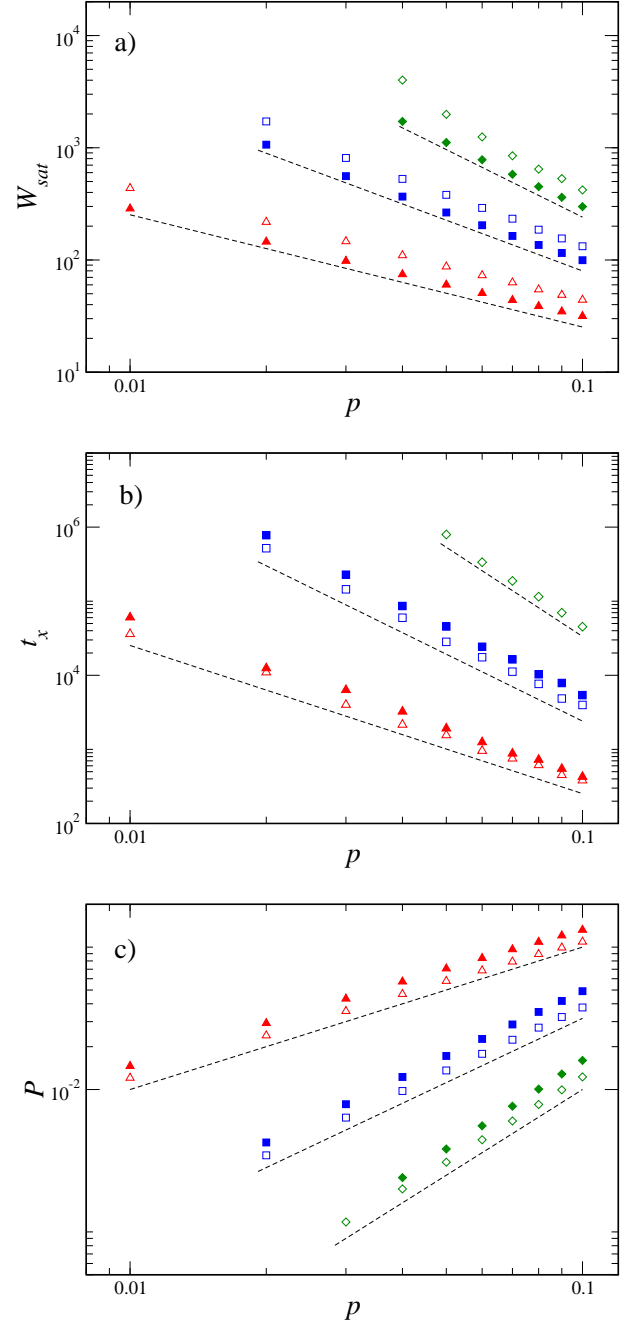


FIG. 4: a) Saturation roughness W_{sat} , b) crossover times t_x and c) porosity P versus probability p for the BBBDS models with $n = 1$ (red triangles), $n = 2$ (blue squares) and $n = 3$ (green diamonds). Data for simulations on $d = 1 + 1$ substrates (open symbols) of size $L = 128$ and $d = 2 + 1$ (full symbols) with $L = 32$ (for $n = 1$ and 2) and $L = 16$ ($n = 3$) are shown. In order to improve visualization, in (c) the data for $d = 2 + 1$ are divided (shifted down) by 1.4. The straight lines have slopes (from the bottom to top): a) -1 , $-3/2$ and -2 , b) -2 , -3 and -4 , and c) 2 , $3/2$ and 1 .

able to obtain the exponent y directly from the t_x scaling. However, since $\Delta = y - \delta$, from the Δ and δ exponents

	BBBDS1	BBBDS2	BBBDS3
y	2.01(4)	3.04(5)	4.0(1)
δ	0.99(1)	1.50(2)	2.0(1)
Δ	0.98(4)	1.49(2)	1.98(3)
y	2.1(1)	3.05(5)	--
δ	0.97(4)	1.50(2)	1.93(5)
Δ	0.99(3)	1.52(2)	2.02(4)

TABLE II: Amplitude exponents y and δ and porosity exponent $\Delta = y - \delta$ for $d = 1 + 1$ (top) and $d = 2 + 1$ (bottom).

we obtain $y \approx 3.95$.

V. DISCUSSIONS AND CONCLUSIONS

We have studied ballistic-like models where bond break of suspended particles is allowed (the BBBD models). The competition between RD-like and DB-like depositions in these models produces a crossover from random to KPZ growth in the temporal evolution of the surface roughness that follows the same scaling relation observed in previous models with random to correlated growth. Using scaling arguments we show that the exponents describing the roughness and crossover time amplitudes, for the BBBD models, are $\delta = (n + 1)/2$ and $y = (n + 1)$, where n is either the maximal number of bonds broken or of suspended particles dislodged. Such exponents are confirmed by numerical simulations of the models on one- and two-dimensional substrates (sumarized in Tables I and II) and they are expected to hold in any dimension. These results generalize the classification present in literature, where models with random-to-correlated competition were divided in two groups: solid-on-solid ones, with

$\delta = 1$ and $y = 2$, and ballistic-like ones, where $\delta = 1/2$ and $y = 1$. In fact, this exponents are not universal, as claimed in previous works, and in ballistic-like models we must have the general exponents found here (Eq. 2). These exponents reduces to $\delta = 1/2$ and $y = 1$ if $n = 0$, i. e., if there is no bond breaking, as considered in previous works.

Models accounting for the maximal number of bonds breaking (BBBDB) and for the maximal number of suspended particles dislodged (BBBDS) have different rates of particle dislodgement, what leads to large differences in crossover times, saturation roughness and porosity. However, they have the same exponents (given by Eq. 2), showing that these ones are independent of some details of the model and must be observed when n particles can be dislodged in a column. In fact, in Fig. 1 we see that in both classes of models up to n suspended particles in a column could be dislodged, but in the BBBDB models these particles sometimes do not move because they have lateral neighbors, and thus a large number of bonds.

Finally, we showed that the bulk porosity P of the deposit is related with the probability p (for small p) through the surface exponents discussed above, with $P \sim p^{y-\delta}$. This scaling relation was confirmed with numerical simulations on $d = 1 + 1$ and $d = 2 + 1$ substrates, and must be valid in any substrate dimension. It also explains the relation $P \sim p^{1/2}$ found for the bidisperse BD model in [27], and it must works in any system with random-to-correlated crossover forming a porous deposit.

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